Supporting Information

Exploration of One-Dimensional Iron-Based Coordination Polymer for

Enhanced Lithium Storage Capabilities

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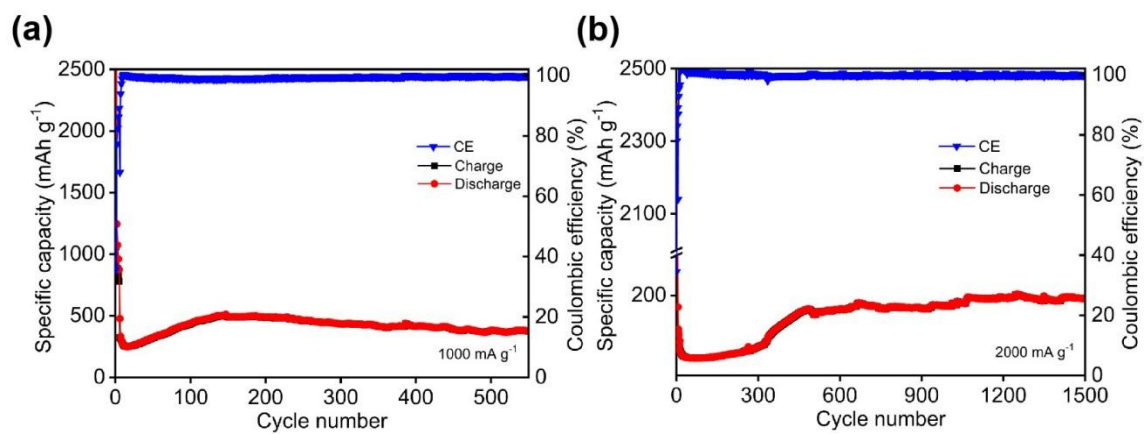Binzhou, 256606, Shandong, China.

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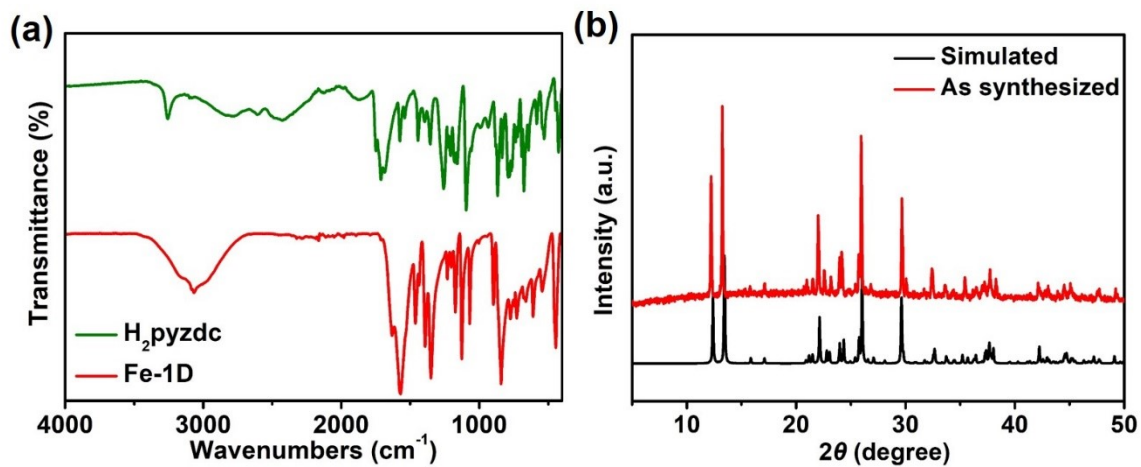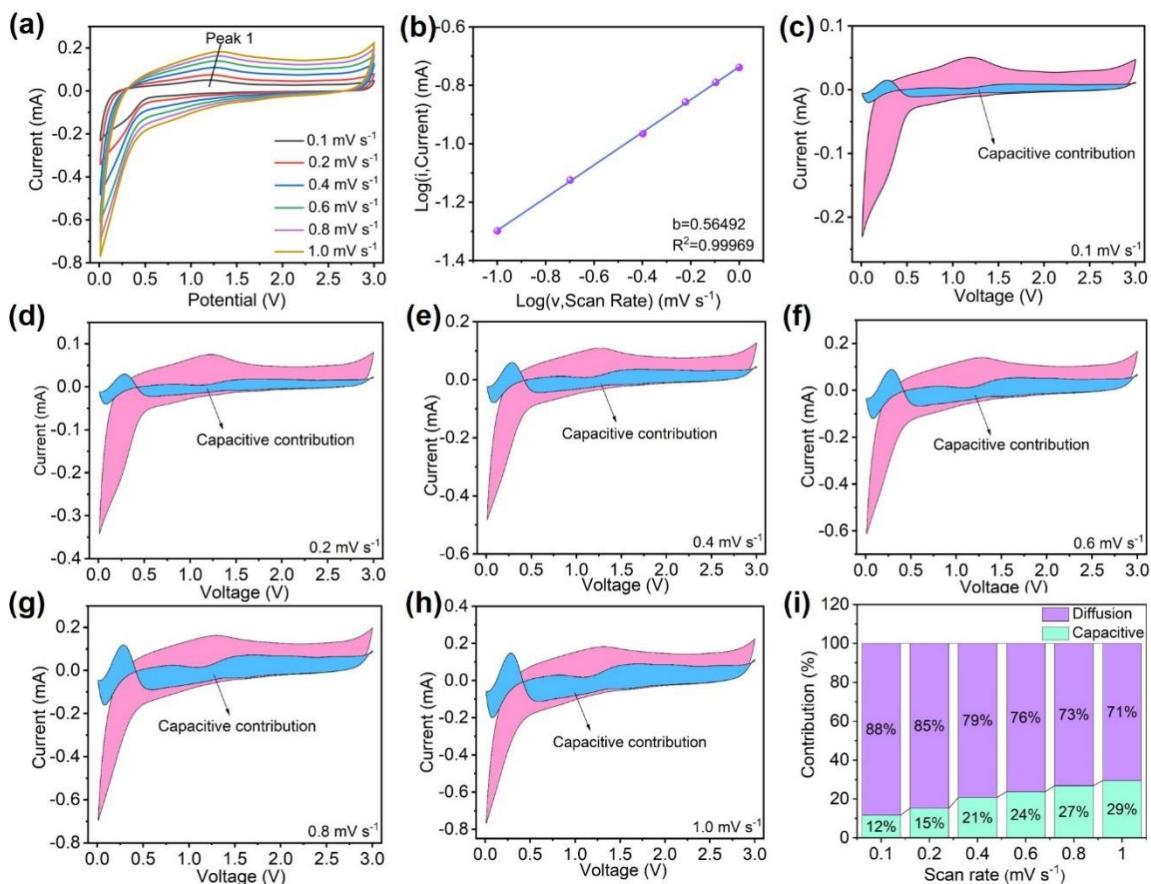
Figure S1. (a) Infrared spectra of Fe-1D, (b) PXRD of Fe-1D.
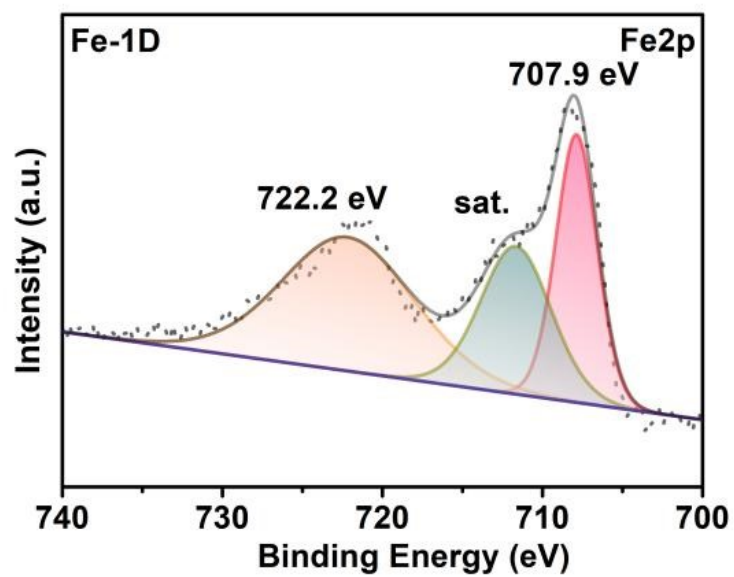
Figure S2. Fe 2p high-resolution XPS spectrum of Fe-1D.

Figure S3. (a) Charge-discharge profiles at 1000mA g^{-1}, (b) Charge-discharge profiles at

2000mA g^{-1}.

Figure S4. (a) CV curves at different scan rates of Fe-1D, (b) Log (i) vs log (v) plots at specific peak current of Fe-1D, (c-h) Pseudo-capacitance control contribution at 0.1, 0.2, 0.4, 0.6, 0.8, 1.0 mV·s^{-1} as a percentage of the total capacity contribution of Fe-1D, (i) The relative contributions of pseudocapacitive capacities and diffusion-controlled capacities at various scan rates.
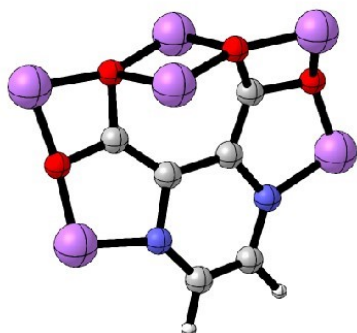
(a)　　　　　　　　　**(b)**
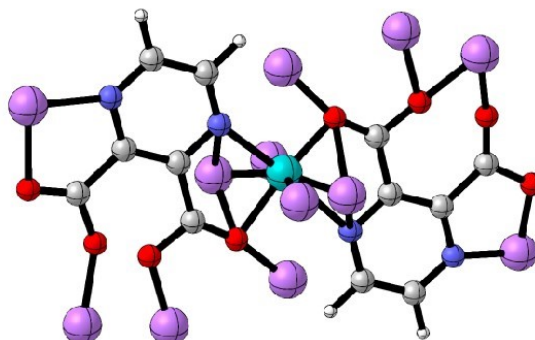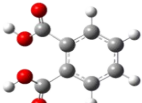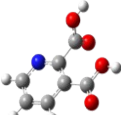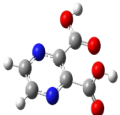
Figure S5. Theoretical lithium storage sites of (a) 2,3-Pyrazinedicarboxylicacid and (b)

Fe-1D.

Figure S6. (a) Density of states (DOS) and (b) Electronic band structure of Fe-1D.

Table S1. Calculated theoretical capacities and LUMO/HOMO energy levels of the selected aromatic ligands
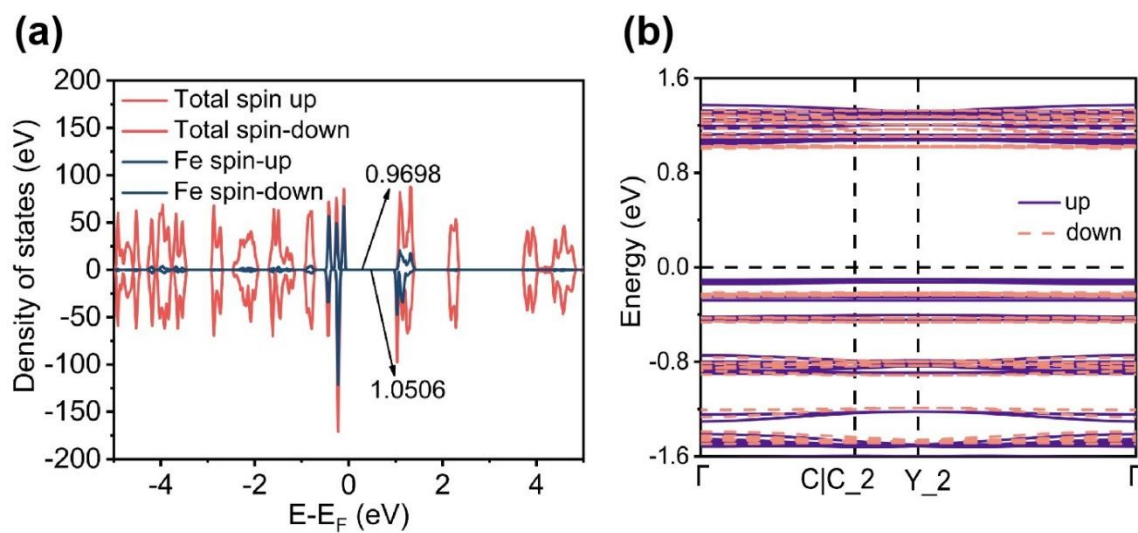
Structure						
Molecular formula	C_6H_6O	C_7H_6O	$C_7H_6O_2$	$C_8H_6O_4$	$C_7H_5NO_4$	$C_6H_4N_2O_4$
Theoretical number of Li uptake	1	1	2	4	5	6
Theoretical Capacity (mAh g^{-1})	285	253	439	646	801	956
LUMO (Hartree)	-0.002	-0.069	-0.057	-0.069	-0.076	-0.099
HOMO (Hartree)	-0.242	-0.257	-0.265	-0.277	-0.279	-0.268
Energy level gap (eV)	6.53	5.11	5.66	5.64	5.52	**4.6**

1 Hartree = 27.211386230 eV

Table S2. Crystallographic data and refinement parameters

Empirical formula	$C_{12}H_8FeN_4O_{10}$
Formula weight	424.07
Temperature/K	298
Crystal system	monoclinic
Space group	I2/a
a/Å	14.9219(19)
b/Å	8.4923(7)
c/Å	13.0852(17)
$\alpha/°$	90
$\beta/°$	118.145(17)
$\gamma/°$	90
Volume/Å^3	1462.1(4)
Z	4
ρcalcg/cm^3	1.927
μ/mm-1	1.104
F(000)	856
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.71 to 52.994
Index ranges	$-17 \leq h \leq 18, -10 \leq k \leq 10, -15 \leq l \leq 16$
Reflections collected	4511
Independent reflections	1515 [R_{int}= 0.0385, R_{sigma}= 0.0701]
Data/restraints/parameters	1515/0/126
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1= 0.0465, wR_2= 0.1151
Final R indexes [all data]	R_1= 0.0707, wR_2= 0.1241
Largest diff. peak/hole / e Å^{-3}	0.54/-0.53

Table S3. The hydrogen bond parameters

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	D-H-A (°)
O(4)-H4···O(5)	0.82	1.69	2.489	166
O(5)-H5A···O(1)	0.85	1.72	2.524	158
O(5)-H5B···N(2)	0.85	1.91	2.755	174

Table S4. The simulated values for impedance spectra before and after 140 cycles

Sample	R_1	R_2	C_1	R_{ct}	C_2	W_{1-R}	W_{1-T}	W_{1-P}
As assembled	4.385	63.3	7.69×10^{-7}	307	2.81×10^{-6}	36.53	0.60	0.37
After 140 cycles	10.04	12.75	6.43×10^{-7}	20.21	2.77×10^{-5}	20.39	0.43	0.37

Table S5. Cartesian coordinates for 2,3-Pyrazinedicarboxylicacid lithium storage.

Element	Coordinates			Element	Coordinates		
	X	Y	Z		X	Y	Z
C	-0.608466	-2.765617	0.209386	O	2.985352	0.660865	-0.222401
C	0.699153	-2.758312	-0.187117	C	-1.611892	0.625924	-0.243653
N	1.420167	-1.570464	-0.255792	O	-2.994979	0.462525	-0.101306
C	0.767202	-0.376939	-0.115026	O	-1.314437	2.020576	-0.405093
C	-0.715961	-0.382383	0.050323	Li	0.385661	2.340653	-0.969262
N	-1.337848	-1.625766	0.423026	Li	2.967953	1.938533	1.003171
H	-1.123887	-3.705771	0.384596	Li	-3.120411	2.208651	-0.413433
H	1.247454	-3.674345	-0.365935	Li	-0.437502	1.724761	-0.413433
C	1.563023	0.799907	-0.230478	Li	3.203638	-1.053584	-0.413433
O	1.216778	1.983109	0.632961	Li	-3.132627	-1.198476	-0.413433

Table S6. Cartesian coordinates for Fe-1D lithium storage.

Element	Coordinates			Element	Coordinates		
	X	Y	Z		X	Y	Z
C	-4.267539	0.617647	0.004618	O	-3.332715	-2.029725	-0.078487
C	2.876032	-0.352126	0.096159	C	-5.30412	-0.540792	0.046475
N	1.964415	-1.344018	0.160857	O	-5.137745	-1.759744	0.040299
C	2.449187	-2.602284	0.133645	O	-6.577726	-0.079846	0.129339
C	3.840711	-2.867823	0.042089	C	5.298484	0.524018	-0.068557
N	4.752274	-1.875946	-0.022606	O	6.52524	0.479355	-0.150018
H	1.711046	-3.419737	0.186068	O	4.714157	1.748277	-0.034499
H	4.227932	-3.900023	0.020451	Fe	0.068356	-0.154514	0.028234
C	2.335219	1.089474	0.126361	Li	-1.225114	0.099533	1.066233
O	1.177836	1.499772	0.201739	Li	1.525839	0.181283	-0.914471
O	3.327045	2.012957	0.056575	Li	-0.099004	-0.102382	-1.428999
C	-2.454845	2.585531	-0.155768	Li	0.255011	0.129689	1.655052
C	-3.846357	2.851053	-0.064227	Li	-2.617331	-3.778632	-0.119494
N	-4.757974	1.859416	0.000471	Li	0.157802	-2.625928	-0.662981
C	-4.273202	0.600894	-0.026741	Li	2.611648	3.761864	0.097151
C	-2.881678	0.335356	-0.118297	Li	-0.330886	2.510181	0.129655
N	-1.970115	1.327232	-0.182992	Li	-4.516662	-3.418516	0.524054
H	-1.716687	3.402971	-0.208162	Li	4.869813	3.758316	0.118641
H	-4.233577	3.883233	-0.042602	Li	6.812142	-1.608313	0.019293
C	-2.340875	-1.106247	-0.148517	Li	-6.637758	1.777408	-0.186783
O	-1.183495	-1.516551	-0.223908				

Table S7. The basic electrochemical properties of the Fe-based anode materials.

Electrode materials	Capacity (mAh g^{-1})	Current density (mA g^{-1})	Cycle number	Voltage (V)	Refs
Fe-ZIF@C	719	100	100	0.01-2.5	1
Fe$_3$O$_4$@C	570	100	60	0.01-3	2
[Fe(C$_5$O$_5$)(H$_2$O)$_3$]$_n$ **(1D)**	521	100	140	0.01-2.4	3
Ti$_{0.9}$Fe$_{1.1}$O$_3$	454.9	100	500	0.01-2.5	4
Fe$_3$O$_4$/GN (15%)	825	100	100	0.01-3	5
MIL-88B(Fe)	189	200	100	0.1-3	6
Fe$_2$(SO$_4$)$_3$	540	1000	100	0.01-3	7
Fe$_3$O$_4$@CTP QDs-2	810	100	200	0.01-3	8
Fe$_3$O$_4$	108	100	200	0.01-3	
semi-crystalline Fe-MOF	854	85	100	0.01-3	9
Fe-1D	833	200	300	0.01-3	this work

Theoretical methods and computational details:

Band structure analysis and the corresponding projected density of states (PDOS) calculations for Fe-1D were conducted using the Vienna Ab initio Simulation Package (VASP).[10,11] For the electronic structure calculations, the Generalized Gradient Approximation (GGA) in conjunction with the Perdew-Burke-Ernzerhof (PBE) functional[12] was employed. The kinetic energy cut-off was set to 400 eV, and the K-point mesh was configured as 2 x 3 x 2. The optimization process was terminated when both the energy and force criteria converged to 1.0×10^{-5} eV and 0.02 eV/Å, respectively.

Calculations pertaining to HOMO/LUMO and ESP for both H2pyzdc and Fe-1D were executed using Gaussian 16 software.[13] Geometric optimization and frequency analysis were carried out employing the B3LYP functional, in conjunction with a hybrid basis set: SDD for Co and Ni atoms,[14] and 6-311+G(d)[15] for C, H, N, and O atoms.

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